

Accurate evaluations of the field shift and lowest-order QED correction for the ground 1^1S -states of some light two-electron ions.

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Abstract

Mass-dependent and field shift components of the isotopic shift are determined to high accuracy for the ground 1^1S -states of some light two-electron Li^+ , Be^{2+} , B^{3+} and C^{4+} ions. To determine the field components of these isotopic shifts we apply the Racah-Rosental-Breit formula. We also determine the lowest order QED corrections to the isotopic shifts for each of these two-electron ions.

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I. INTRODUCTION

In this study we perform highly accurate computations of the isotopic shifts for the ground 1^1S -states of some light two-electron ions: Li^+ , Be^{2+} , B^{3+} and C^{4+} . In atomic and molecular spectroscopy the isotopic shift [1], [2] usually means the difference (or shift) in the total and/or binding energies of the bound states that occurs when one nuclear isotope is replaced by another. It is clear *a priori* that the total energies and other bound state properties of light atoms and ions depend upon the inverse mass of the central nucleus and proton density distribution in that nucleus. In some cases a few other nuclear properties, e.g., the nuclear magnetic moment, also contribute to the total energies of atoms and ions, and therefore, to the isotopic shifts. In this study we perform highly accurate evaluations of the different components of isotopic shifts in the light two-electron ions Li^+ , Be^{2+} , B^{3+} and C^{4+} . Our approach is essentially non-relativistic, i.e. we use the non-relativistic wave functions which are determined as the solutions of the non-relativistic Schrödinger equation for each of these two-electron ions. For heavier two-electron ions, e.g., for the O^{6+} , F^{7+} and Ne^{8+} ions, the contribution of the relativistic and QED corrections rapidly increases with the nuclear charge Qe (or Q) and isotopic shifts for such ions can be determined to high accuracy only with the use of the relativistic bi-spinor wave functions which must be obtained from the Dirac equation(s). The wave functions arising from the non-relativistic Schrödinger equation can be applied to such heavy two-electron ions to determine only approximate values of some lowest-order relativistic and QED-corrections.

In this study numerical evaluations of the isotopic shifts in light atoms and ions are based on highly accurate computations of the expectation values of a few selected electron-nuclear and electron-electron operators. At the first stage of our procedure we apply the wave functions which have been determined for model ions which have an infinitely heavy nucleus. By using these wave functions we determine the expectation values of operators which are included in different components of the isotopic shift. Formally, these expectation values allow us to evaluate the isotopic shifts (in the lowest-order approximation and to relatively high accuracy) for the ground states of all two-electron ions considered in this study (i.e. in the Li^+ , Be^{2+} , B^{3+} and C^{4+} ions). However, the overall accuracy of our evaluations can be drastically improved, if we determine the same expectation values and the total energies for the two-electron ions with finite-mass nuclei. Indeed, each atomic

system includes a central atomic nucleus and the mass of such a nucleus is always finite. An error in the total energy due to replacement of the actual, finite mass nucleus by an infinitely heavy nucleus can be evaluated as $\approx 1 \cdot 10^{-6} - 1 \cdot 10^{-5} \text{ a.u.}$ For other bound state properties which can also contribute to various corrections to the total energy such (relative) errors vary between $\approx 1 \cdot 10^{-7}$ and $\approx 1 \cdot 10^{-3}$. Furthermore, there are additional corrections related to the fact that all nuclear masses are known only approximately. In reality, this means that all nuclear masses are the subject to constant experimental revision. It is clear that to solve the problem of isotopic shift completely we need to determine the mass gradients for each of the expectation values used to evaluate the isotope shifts in the same two-electron ions with varying nuclear masses.

This work has the following structure. Representation of the isotopic shift in atoms as the sum of its leading components is discussed in Section II. In that Section we also investigate the formula which is used to determine the field component of the isotopic shift. Calculations of isotopic shifts for some light two-electron ions are performed in Section III, namely for the ground 1^1S -states in the Li^+ , Be^{2+} , B^{3+} and C^{4+} ions with an infinitely heavy central nucleus. Here we also discuss a system of tests for the non-relativistic wave functions which can be used in actual calculations. Section IV contains results of highly accurate computations for the two-electron ions with the finite nuclear masses. This Section is a central part of our study. Section V contains formulas for calculation of the lowest order QED correction in two-electron ions. Concluding remarks can be found in the last Section.

II. COMPONENTS OF THE ISOTOPIC SHIFT

In general, the isotopic shift ΔE of the bound state level with the total energy E can be represented as the sum of a few different components. In many cases the two largest components in such sums are: (a) the mass component ΔE_M , which explicitly depends on the mass of the central nucleus, and (b) the field shift component ΔE_F , which mainly depends upon the electric charge distribution in the atomic nucleus. The first component ΔE_M is represented as the sum of the normal and specific components. Each of these two components is proportional to the factor $\frac{m_e}{M}$, where m_e is the mass of the electron at rest, while M is the nuclear mass (at rest) expressed in m_e . For few-electron (N -electron) atoms

and ions the exact formula for the isotopic shift ΔE_M takes the form (see, e.g., [3])

$$\Delta E_M = \Delta E_M^{nms} + \Delta E_M^{sms} = \frac{m_e}{M} \left\langle \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m_e} \right\rangle + \frac{m_e}{M} \left\langle \sum_{i(i \geq k)=2}^N \sum_{k=1}^{N-1} \frac{\mathbf{p}_i \cdot \mathbf{p}_k}{2m_e} \right\rangle \quad (1)$$

where ΔE_M^{nms} is the normal mass shift, ΔE_M^{sms} is the specific mass shift and the notation $\langle \hat{X} \rangle$ designates the expectation value of the operator \hat{X} . For the two-electron (or helium-like) atoms and ions the expressions for the normal and specific components of the isotope shift are

$$\Delta E_M^{nms} = \frac{1}{M} \langle \mathbf{p}_1^2 \rangle \quad \text{and} \quad \Delta E_M^{sms} = \frac{1}{2M} \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \quad , \quad (2)$$

respectively. As follows from Eq.(2), to determine the normal and specific components in two-electron atom/ion one needs to obtain the expectation values of the \mathbf{p}_1^2 and $\mathbf{p}_1 \cdot \mathbf{p}_2$ operators. Everywhere in this study we assume that the wave functions of the two-electron atom/ion are properly symmetrized upon spin-spatial permutations of the two electrons and, therefore, the corresponding single-electron expectation values are always equal to each other, e.g., $\langle \mathbf{p}_1^2 \rangle = \langle \mathbf{p}_2^2 \rangle$.

In actual two-electron ions and atoms, i.e. in atomic systems with the finite nuclear mass M , one can use the condition which follows from the conservation of the total momentum $\mathbf{P}_N = \mathbf{p}_1 + \mathbf{p}_2$, where \mathbf{P}_N is the momentum of the nucleus, while \mathbf{p}_1 and \mathbf{p}_2 are the electron momenta. From here one finds:

$$\frac{1}{2} \langle \mathbf{P}_N^2 \rangle = \langle \mathbf{p}_1^2 \rangle + \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \quad (3)$$

and, therefore, from Eq.(1) for $N = 2$ and Eq.(3) we obtain

$$\Delta E = \frac{1}{2M} \langle \mathbf{P}_N^2 \rangle \quad (4)$$

i.e. the mass-dependent component of the isotopic shift is the expectation value of the kinetic energy of the atomic nucleus with the finite mass. In many books and textbooks the formula, Eq.(4), is considered as the original (or fundamental) expression, while Eq.(1) is derived from this formula.

A. The field component of the isotope shift

In contrast with the mass component ΔE_M , Eq.(4), the field component of the isotopic shift ΔE_F explicitly depends upon the nuclear size (or nuclear radius) R and proton density

distribution in that nucleus. It is clear that this component also depends upon the nuclear mass M , since nuclear matter is a saturated matter (in contrast with Coulomb matter). The nuclear radius R is uniformly related to the number of nucleons A in the nucleus: $R = r_0 \cdot A^{\frac{1}{3}}$, where the ‘constant’ radius is $r_0 \approx 1.17 - 1.25 \cdot 10^{-13} \text{ cm} = 1.17 - 1.25 \text{ fm}$ (fermi), where $1 \text{ fm} = 1 \cdot 10^{-13} \text{ cm}$. Briefly, this means that the field component of the total isotopic shift is also a function of the nuclear mass M , since $A \approx \frac{M}{m_p}$, where m_p is the proton mass. In general, the nuclear mass is a function of $A, Z(= N_p)$, where Z is the electric charge of the nucleus = number of protons N_p , and N_n is number of neutrons. The formula for $M(A, Z)$ is known as the Weizäcker formula. This formula is discussed in the Appendix.

The field component of the isotopic shift ΔE_F is determined by the expression which is widely known as the Racah-Rosental-Breit formula (see, e.g., [1] and references therein). In atomic units ($\hbar = 1, e = 1, m_e = 1$) this formula takes the form

$$\Delta E_F = \frac{4\pi a_0^2}{Q} \cdot \frac{b+1}{[\Gamma(2b+1)]^2} \cdot B(b) \cdot \left(\frac{2QR}{a_0}\right)^{2b} \cdot \frac{\delta R}{R} \cdot \langle \delta(\mathbf{r}_{eN}) \rangle \quad (5)$$

where Q is the nuclear charge, R is the nuclear radius and $b = \sqrt{1 - \alpha^2 Q^2}$, where $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the dimensionless constant which is the small parameter in QED. In Eq.(5) the notation $\Gamma(x)$ stands for the Euler’s gamma-function, while the factor $B(b)$ is directly related to the proton density distribution in the atomic nucleus. By assuming a uniform distribution of the proton density over the volume of the nucleus one finds the following expression for the factor $B(b)$

$$B(b) = \frac{3}{(2b+1)(2b+3)} \quad (6)$$

For light nuclei with $Q \leq 6$ we have $b \approx 1$ and $B \approx \frac{1}{5}$. The formula, Eq.(5), has been used in many papers for numerical evaluations of the field component of the isotopic shift, or field shift, for short. In some works, however, this formula was written with a number of ‘obvious simplifications’. Many such ‘simplifications’ are based on the fact that for light nuclei the numerical value of the factor b is close to unity. Furthermore, in some papers the factor b was mistakenly called and considered as the Lorentz factor, while the actual Lorentz factor γ is the inverse value of b , i.e., $\gamma = \frac{1}{b} = \frac{1}{\sqrt{1 - \alpha^2 Q^2}}$, which always exceeds unity. As follows from Eq.(5) in order to determine the field component of the isotopic shift in light atoms one needs to know the radius of the nucleus R and the expectation value of the electron-nucleus delta-function $\langle \delta(\mathbf{r}_{eN}) \rangle$.

In this study we evaluate the field components of the isotopic shift for a number of the ground $1^1S(L = 0)$ -states in light two-electron ions by using the exact formula, Eq.(5). This allows one to evaluate the numerical errors which arise from the use of approximate expressions. As follows from Eq.(5), to evaluate the field component of the field shift one needs to determine to very high accuracy the expectation value of the electron-nuclear delta-function, i.e. $\langle \delta(\mathbf{r}_{eN}) \rangle$. In the lowest-order approximation the ratio $\frac{\delta R}{R}$ in Eq.(5) can be assumed to be equal unity. The formula for ΔE_F is reduced to the form (in atomic units)

$$\Delta E_F = 4^{b+1} \pi Q^{2b-1} \cdot \alpha^{4b} \cdot \frac{3(b+1)}{[\Gamma(2b+1)]^2 (2b+1)(2b+3)} \cdot \left(\frac{R}{r_e}\right)^{2b} \cdot \langle \delta(\mathbf{r}_{eN}) \rangle \quad (7)$$

where $r_e = \alpha^2 a_0 \approx 2.817940 \text{ fm}$ ($1 \text{ fm} = 1 \cdot 10^{-13} \text{ cm}$ is one *fermi*) is the classical radius of the electron. For atomic nuclei the dimensionless factor $\frac{R}{r_e}$ in the last formula is close to unity. Also, in our calculations we have used the following numerical values for the physical constants: $\alpha = 7.2973525698 \cdot 10^{-3}$ and $a_0 = 5.2917721092 \cdot 10^{-9} \text{ cm}$. The formula, Eq.(7), has been used in all calculations of ΔE_F performed in this study. As follows from Eq.(7) to determine the field component of the isotopic shift one needs to know the expectation value of the electron-nuclear delta-function $\delta(\mathbf{r}_{eN})$ and numerical value of the nuclear radius R . The expectation value $\langle \delta(\mathbf{r}_{eN}) \rangle$ can be found from the results of highly accurate atomic computations, while the nuclear radii of different light nuclei must be taken from nuclear experiments (see, e.g., [4]).

III. BOUND STATE CALCULATIONS OF THE TWO-ELECTRON IONS

Our method used in this study to evaluate different components of the isotopic shift and the lowest-order QED corrections is based on numerical, highly accurate computations of expectation values of some operators. In such calculations we apply the non-relativistic wave functions of the two-electron ions, which are obtained as the solutions of the Schrödinger equation [3] for the bound states $H\Psi = E\Psi$, where $E < 0$ and H is the non-relativistic Hamiltonian of the two-electron ions

$$H = -\frac{\hbar^2}{2m_e} (\nabla_1^2 + \nabla_2^2 + \frac{m_e}{M_N} \nabla_N^2) + \frac{Qe^2}{r_{32}} + \frac{Qe^2}{r_{31}} + \frac{e^2}{r_{21}} \quad (8)$$

where $\nabla_i = \left(\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i} \right)$ and $i = 1, 2, 3 (= N)$, where the notation $N (= 3)$ stands for the nucleus. In Eq.(8) the notation \hbar stands for the reduced Planck constant, i.e. $\hbar = \frac{h}{2\pi}$, and

e is the elementary electric charge. Everywhere below in this study the particles 1 and 2 mean the electrons, while the particle 3 is the atomic nucleus with the mass $M_N \gg m_e$. The dimensionless ratio $\tau_m = \frac{m_e}{M_N}$ is the small parameter of the method. For light atoms it is very convenient to perform all bound state calculations in atomic units in which $\hbar = 1, m_e = 1$ and $e = 1$. In these units the velocity of light in vacuum c numerically coincides with the inverse value of the dimensionless fine structure constant, i.e. $c = \alpha^{-1}$, where $\alpha = \frac{e^2}{\hbar c} \approx 7.2973525698 \cdot 10^{-3} \approx 1/137.035999074$ is the fine structure constant [5]. In atomic units the same Hamiltonian, Eq.(8), is written in the form

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2 + \frac{1}{M_N}\nabla_3^2) - \frac{Q}{r_{32}} - \frac{Q}{r_{31}} + \frac{1}{r_{21}} \quad (9)$$

It should be emphasized that our approach based on the use of non-relativistic wave functions will work, if (and only if) the non-relativistic variational wave functions have been determined to very high accuracy (precise wave functions). For the ground $1^1S(L=0)$ -states of the light two-electron ions the highly accurate wave functions are approximated with the use of the exponential variational expansion in relative coordinates r_{32}, r_{31} and r_{21} (see, e.g., [6] and references therein)

$$\Psi = \left(1 + \hat{P}_{12}\right) \sum_{i=1}^N C_i \exp(-\alpha_i r_{31} - \beta_i r_{31} - \gamma_i r_{21}) \quad (10)$$

Each of these three relative coordinates r_{ij} is defined as the difference between the corresponding Cartesian coordinates of the two particles, e.g., $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, where \mathbf{r}_i and \mathbf{r}_j are the Cartesian coordinates of particles i and j . It follows from this definition that the relative coordinates r_{32}, r_{31} and r_{21} are translationally and rotationally invariant. The coefficients C_i are the linear (or variational) parameters of the variational expansion, Eq.(10), while the parameters α_i, β_i and γ_i are the non-linear (or varied) parameters of this expansion. To optimize such non-linear parameters in Eq.(10) we have developed a very effective two-stage optimization strategy [6]. The operator \hat{P}_{12} in Eq.(10) is the permutation operator for two identical particles (electrons).

In this study we consider several light two-electron (or He-like) ions: Li^+ , Be^{2+} , B^{3+} and C^{4+} . Our results given in Tables I - IV allow one to determine the normal and specific components of the isotopic shifts ΔE_M in these cases. Furthermore, by using the expectation value of the electron-nucleus delta-functions in each of these ions one can determine the corresponding field shifts ΔE_F (see Table V). Formally, our data from Tables I - V contain

all expectation values which are needed to determine the numerical values of ΔE_M and ΔE_F . All data presented in these Tables correspond to the two-electron ions with infinitely heavy nuclei. The significance of the computed components of the isotopic shift (ΔE_M and ΔE_F) in actual applications can be reliably determined, if we can evaluate the same expectation values for the atoms/ions with the finite nuclear masses. This problem is discussed in Section IV.

Here we want to consider another problem which arises during numerical evaluation of the ΔE_M and ΔE_F components by using our formulas. Indeed, as we mentioned above, numerical evaluations of the isotope shifts in these two-electron ions is reduced to highly accurate calculations of the expectation values of some electron-nucleus and electron-electron operators, which include the inter-particle delta-functions. The overall accuracy of these expectation values is a crucial question for highly accurate evaluations of the isotope shifts. In turn, this is directly related to the overall accuracy of the wave functions used in calculations. Since the early years of quantum mechanics the accuracy of the variational wave functions has been assessed by minimizing the total energy computed with such a wave function. This simple ‘criterion of the quality’ does not work for the expectation values of operators which are needed to determine the isotopic shifts in light ions/atoms. Indeed, currently by using a number of special methods, e.g., GFMC method (or Green Function Monte-Carlo method), it is easy to construct bound state wave functions which produce ‘essentially exact’ total energies for different few-body systems, but the expectation values of some other properties computed with such wave functions are relatively inaccurate. In particular, it is difficult to determine highly accurate expectation values of the electron-nucleus and electron-electron delta-functions, i.e. the local properties, or properties determined at one spatial point. Therefore, below we need to discuss numerical criteria that are used to judge the overall quality of the wave functions and allow us to evaluate the applicability of these wave functions for accurate numerical computations of all interparticle delta-functions and other local properties some of which also include spatial derivatives of different orders. The second closely related question is the convergence rate (upon the total number N of basis functions used) for the expectation values which are needed for numerical evaluation of the isotope shifts. These two questions are considered in this Section.

A natural criterion of the quality of the wave functions which was used already in the first variational calculations of atomic and molecular systems is based on the virial theorem

(see, e.g., [7]). The virial theorem for Coulomb systems, e.g., for atoms and ions, can be written in the form $2\langle T \rangle = -\langle V \rangle$, where T is the operator of the kinetic energy and V is the operator of the potential energy. Since the Hamiltonian H is represented as the sum $H = T + V$, then one finds for the expectation values $\langle H \rangle = E = -\langle T \rangle = \frac{1}{2}\langle V \rangle$, where E is the total energy of the atomic system bound by the Coulomb interparticle potentials. In general, this criterion is simple, but in many cases is not sufficient to evaluate the overall quality of the variational wave functions which then can be used for various purposes, e.g., to determine the expectation values of different quantum operators. It is clear that some other criteria are needed. Fortunately, for all Coulomb few-body systems we can always evaluate (exactly) the particle densities at the two-particle coalescence points. For instance, for the three-particle (or two-electron) ions Li^+ , Be^{2+} , B^{3+} and C^{4+} we have two such a coalescence points: the electron-nucleus point and electron-electron point. At each of these points we can calculate the expectation values of the following operators (or cusp-operators)

$$\nu_{eN} = \frac{\langle \delta(\mathbf{r}_{eN}) \frac{\partial}{\partial r_{eN}} \rangle}{\langle \delta(\mathbf{r}_{eN}) \rangle} \quad (11)$$

in the case of the electron-nucleus cusp, and

$$\nu_{ee} = \frac{\langle \delta(\mathbf{r}_{ee}) \frac{\partial}{\partial r_{ee}} \rangle}{\langle \delta(\mathbf{r}_{ee}) \rangle} \quad (12)$$

for the electron-electron cusp. These two expectation values must coincide with the known values of these cusps, i.e., with the following numerical values (in atomic units)

$$\nu_{eN} = -Qe^2 \frac{m_e M_N}{m_e + M_N} = -Q \frac{1}{1 + \frac{1}{M_N}} = -Q(1 + M_N^{-1})^{-1} \quad , \quad \nu_{ee} = 0.5 \quad (13)$$

where $M_N = \frac{M_N}{m_e}$ is the nuclear mass which can be finite (real), or infinite for model atomic systems.

The coincidence of these two expectation values, Eqs.(11) - (12), with the predicted values, Eq.(13), is a very effective test for the variational wave functions in any Coulomb system. In real applications, however, different authors try to ‘improve’ their actual cusp values using various tricks, e.g., by adding additional ‘special’ terms to the wave functions. These additional terms do not change the computed variational energy, but they allow one to obtain ‘very accurate’ cusps. Such results are published by some authors to support claims of extremely high quality of variational wave functions. In general, at this moment it is hard to trust such results without investigating expectation values of other quantum operators.

On the other hand, for each of the two-electron atoms and ions (at least, for their ground and low-excited states) one finds in the literature a large number of expectation values already computed to high numerical accuracy. Formally, all conclusions about the overall quality of the three-particle wave function must follow from numerical comparison of the computed expectation values and values known from the literature. Ideally, such a complete set of required expectation values includes not only regular expectation values, but singular expectation values too. For actual two-electron ions (and, in general, for few-electron atomic systems) it is possible to find a few such properties (or ‘complex’ expectation values) which include the expectation values of all delta-functions and at least one singular expectation value. Accurate numerical computations of this set of expectation values provide a very effective criterion for the overall quality of the wave function used.

In reality, a number of such criteria for the quality of the variational wave functions used in calculations can be found among various lowest-order relativistic and QED corrections. Indeed, these corrections contain singular expectation values and different interparticle delta-functions. By determining these corrections and comparing results with the known numerical values one can estimate the quality of the trial wave functions. In particular, below we determine the lowest-order QED correction for each of the two-electron ions considered. However, at the first stage of our calculations we apply the electron-nuclear and electron-electron cusps as criteria of the quality of our wave functions.

In this study we determine both the electron-nucleus and electron-electron cusp values and compare them with the known (or expected) cusps, i.e., with $-Q(1 + M_N^{-1})^{-1}$ and 0.5 (in atomic units), respectively. In calculations performed here we have also determined many dozens of other expectation values, including some singular expectation values (see the corresponding Tables in [8]). In general, all these expectation values are very close to the values given in [8], but our current values are more accurate. This means that our wave functions have better numerical accuracy. Numerical values of the particular expectation values (in atomic units) needed for numerical evaluations of the isotopic shifts in the Li^+ , Be^{2+} , B^{3+} and C^{4+} ions with the infinitely heavy nuclei are presented in Tables I - IV, respectively. Expectation values from Tables I - IV include the total energies, electron-nucleus delta-functions and cusp values. Each of these Tables also contain the expectation values $\frac{1}{2}\langle \mathbf{p}_1^2 \rangle$, $\langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle$ and $\frac{1}{2}\langle \mathbf{p}_N^2 \rangle$ which are needed for zero-order evaluation of the isotopic shifts. Based on these results and by applying the formula, Eq.(7), we have determined the

numerical values of the field components of isotopic shifts which are presented in Table V (in atomic units). This Table also includes numerical values of the following factors from the formula, Eq.(7): R (the actual nuclear radius), b , $X = 4^{b+1}\pi Q^{2b-1} \cdot \alpha^{4b} \cdot \frac{3(b+1)}{[\Gamma(2b+1)]^2(2b+1)(2b+3)}$ and $Y = \left(\frac{R}{r_e}\right)^{2b}$. The expectation values of the electron-nuclear delta-functions were taken from Tables I - IV. To evaluate the Euler's gamma-function $\Gamma(x)$ we have used approximate 7-term formula derived by Lanczos [9]. Finally, the overall accuracy of our formula for ΔE_F has been estimated as $\approx 1 \cdot 10^{-10} - 2 \cdot 10^{-10} \text{ a.u.}$

IV. TWO-ELECTRON IONS WITH THE FINITE-MASS NUCLEI

Tables I - V contain results of numerical calculations in which the masses of all atomic nuclei were assumed to be infinite. For light atoms and ions numerical errors related with the finite nuclear masses can be substantial. Even in those cases, when all finite-mass corrections have been evaluated and included in the final formulas one can still identify some numerical errors in the total energies and other properties since such errors can easily be detected in modern highly accurate calculations. Moreover, it is hard to compare directly our computational data obtained for the model ions with infinitely heavy nuclei with the results of precise optical observations performed for actual ions with the finite nuclear masses. The overall accuracy of modern optical experiments based on the use of lasers is already extremely high and continues to increase. Briefly, this means that numerical calculations based on the use of small parameter(s) and perturbation theory lead to a very complex procedure which cannot provide a very high accuracy for the final results. An alternative way is to perform all calculations for the two-electron ions which have the finite nuclear masses from the first step of the procedure. In other words, we need to consider a general three-body problem for Coulomb systems. In this approach we re-calculated the results from Tables I - V for a number of actual ions, i.e. for the Li^+ , Be^{2+} , B^{3+} and C^{4+} ions with the finite nuclear masses. The nuclear masses of the different Li, Be, B and C isotopes used in these calculations are (in atomic units): $M(^6\text{Li}) = 10961.8968 m_e$, $M(^7\text{Li}) = 12786.3927 m_e$, $M(^9\text{Be}) = 16424.2032 m_e$, $M(^{10}\text{Be}) = 18249.5555 m_e$, $M(^{10}\text{B}) = 18247.4677 m_e$, $M(^{11}\text{B}) = 20063.7631 m_e$, $M(^{12}\text{C}) = 21868.66182 m_e$, $M(^{13}\text{C}) = 23697.66580 m_e$ and $M(^{14}\text{C}) = 25520.34677 m_e$. The total energies of these ions with the finite nuclear masses can be found in Table VI.

The expectation values of the operators which are needed to determine the isotopic shifts (or any mass-related shifts) in these two-electron ions can be found in Table VII. These operators are: \mathbf{p}_1^2 , $\mathbf{p}_1 \cdot \mathbf{p}_2$, \mathbf{p}_N^2 and $\delta(\mathbf{r}_{eN})$. For instance, let us assume that in our calculations of some of these two-electron ions we have used the nuclear mass M , while in new experiments it was found that such a mass equals M' . The corresponding correction (or additional mass correction $\Delta_M^{(A)}$) is written in the form

$$\Delta_M^{(A)} = \left(\frac{1}{2M'} - \frac{1}{2M} \right) \langle \mathbf{p}_N^2 \rangle = \left(\frac{1}{M'} - \frac{1}{M} \right) (\langle \mathbf{p}_1^2 \rangle + \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle) \quad (14)$$

where $\langle \mathbf{p}_N^2 \rangle$, $\langle \mathbf{p}_1^2 \rangle$ and $\langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle$ expectation values must be determined for the atomic system with the finite nuclear mass M (i.e. ‘old’ nuclear mass). Analogously, by using the expectation values of the electron-nucleus delta-functions from Table VII one can evaluate the corresponding ‘additional’ field shift $\Delta E_F^{(A)}$ which is related to the ‘new’ nuclear radius R'_N measured in the experiments

$$\Delta E_F^{(A)} = \frac{4\pi a_0^2}{Q} \cdot \frac{b+1}{[\Gamma(2b+1)]^2} \cdot B(b) \cdot \left(\frac{2Q}{a_0} \right)^{2b} \cdot (R' - R) \cdot \langle \delta(\mathbf{r}_{eN}) \rangle \quad (15)$$

where R designates the ‘old’ nuclear radius. In reality, all nuclear radii are currently known to a numerical accuracy $\approx 1 \cdot 10^{-3} \text{ fm}$ (and even better). Therefore, the absolute values of the differences $R' - R$ are very small ($R' - R \leq 1 \cdot 10^{-3} R$ (and smaller)).

The expectation values of operators from Table VII allow one to determine and evaluate the actual and ‘additional’ mass and field shifts for each of the two-electron ions considered in this study. However, for each atomic system one also finds a separate group of small corrections which must be added to the computed total energy, or isotopic shift. One group of such small corrections ($\simeq \alpha^2$) is directly related to the fact that $\frac{v_e}{c}$ is not zero exactly (it is small $\approx 1 \cdot 10^{-5}$, but non-zero!). Another group of small corrections ($\simeq \alpha^3$) to the total energies arises from interaction between atomic electron(s) and radiation quanta. These group of corrections is called the lowest-order QED corrections. These corrections can be determined to high numerical accuracy with the use of a few expectation values computed with the non-relativistic wave functions. Both these corrections are discussed below.

V. RELATIVISTIC CORRECTIONS

The results of highly accurate calculations for two-electron atoms and ions are of great interest by themselves. However, in the Sections above we considered only the non-relativistic

total energies of a few two-electron ions in their ground 1^1S -states. These energies were determined to high numerical accuracy for model ions with the infinitely heavy nuclei and also for actual ions with the finite nuclear masses M_N . It appears that the total energies and all expectation values computed with the non-relativistic wave functions are analytical functions of the dimensionless parameter $\frac{m_e}{M_N} = \frac{1}{M_N}$ which is the inverse mass of the nucleus expressed in the electron mass m_e . In reality, such an idealized picture ignores all lowest-order relativistic and quantum electrodynamic corrections (or QED corrections, for short) for actual two-electron ions. For light two-electron ions these corrections are relatively small $\approx 10^{-3} - 10^{-6} a.u.$ (the overall values are different for different states and ions), but they can be important in some problems. Here we want to restrict our analysis to the lowest-order relativistic ($\simeq \alpha^2$) and QED ($\simeq \alpha^3$) corrections to the energy levels. In this Section we discuss numerical calculations of the lowest-order relativistic corrections. The lowest-order QED corrections are considered in the next Section.

The general theory developed for numerical evaluation of the relativistic corrections in light two-electron atoms and ions can be found in [10] and for many-electron atoms in [3]. For the ground (singlet) 1^1S -states in these ions one finds a number of significant simplifications in the general theory. To simplify our analysis even further here we write only the final formula which is used to determine the lowest-order relativistic correction in the ground singlet state of two-electron atoms/ions. In atomic units this formula takes the form

$$\Delta E_R = -\frac{\alpha^2}{4} \langle \mathbf{p}_1^4 \rangle - \frac{\alpha^2}{2} \langle \frac{1}{r_{12}} \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle - \frac{\alpha^2}{2} \langle \frac{1}{r_{12}^3} \mathbf{r}_{12} (\mathbf{r}_{12} \cdot \mathbf{p}_1) \mathbf{p}_2 \rangle + \pi \alpha^2 [Q \langle \delta(\mathbf{r}_{eN}) \rangle + \langle \delta(\mathbf{r}_{ee}) \rangle] \quad (16)$$

where $\alpha = 7.2973525698 \cdot 10^{-3}$ is the fine-structure constant and Q is the electric charge of the nucleus expressed in terms of the electron charge e . In this equation the particles with indexes 1 and 2 are the electrons, while the particle with index 3 is the atomic nucleus. The notation $r_{ee} = r_{12}$ stands for the electron-electron distance, while the notation $r_{eN} = r_{13}(= r_{23})$ designates the electron-nuclear distance. The formula, Eq.(16), can be used to determine the lowest-order ($\sim \alpha^2$) relativistic correction to the non-relativistic total energies of the ground 1^1S -states in light two-electron ions. For the two-electron ions considered in this study, the last term (i.e. the sum of the expectation values of the delta-functions) in Eq.(16) equals: $3.528190130474 \cdot 10^{-3} a.u.$ for the $^\infty\text{Li}^+$ ion, $1.176338007844 \cdot 10^{-2} a.u.$ for the $^\infty\text{Be}^{2+}$ ion, $2.962880936734 \cdot 10^{-2} a.u.$ for the $^\infty\text{B}^{3+}$ ion and $6.270223554881 \cdot 10^{-2} a.u.$ for the $^\infty\text{C}^{4+}$

ion. The expectation values of other terms from Eq.(16) will be presented elsewhere.

VI. THE LOWEST ORDER QED CORRECTION

As we mentioned above actual calculations of all relativistic and QED corrections in two-electron atoms and ions can be performed only with the use of the truly relativistic wave functions. The non-relativistic wave functions obtained as the solutions of the Schrödinger equation can be applied only for numerical evaluations of some lowest-order relativistic and QED corrections in light two-electron ions. Below, we discuss numerical evaluation of the lowest order QED correction ΔE^{QED} for the two-electron ions: Li^+ , Be^{2+} , B^{3+} and C^{4+} . The corresponding formula for such a correction ΔE^{QED} in a two-electron ion with infinitely heavy nucleus is written in the form (in atomic units)

$$\begin{aligned} \Delta E^{QED} = & \frac{8}{3}Q\alpha^3\left[\frac{19}{30} - 2\ln\alpha - \ln K_0\right]\langle\delta(\mathbf{r}_{eN})\rangle + \alpha^3\left[\frac{164}{15} + \frac{14}{3}\ln\alpha - \frac{10}{3}S(S+1)\right]\langle\delta(\mathbf{r}_{ee})\rangle \\ & - \frac{14}{3}\alpha^3\left\langle\frac{1}{r_{ee}^3}\right\rangle \end{aligned} \quad (17)$$

where α is the fine structure constant, Q is the nuclear charge (in atomic units) and S is the total electron spin. The ground states in all two-electron ions considered in this study are the singlet states with $S = 0$. Also, in this formula $\ln K_0$ is the Bethe logarithm. To determine the Bethe logarithm which is usually evaluated by applying the formula $\ln K_0 = \ln k_0 + 2\ln Q$, where $\ln k_0$ is the charged-reduced Bethe logarithm. Numerical values of the Bethe logarithm were evaluated for each of these two-electron ions (Li^+ , Be^{2+} , B^{3+} and C^{4+}) in earlier works.

The last term in Eq.(17) is called the Araki-Sucher term, or Araki-Sucher correction, since this correction was obtained and investigated for the first time in papers by Araki and Sucher [11], [12]. The expectation value of the term $\langle\frac{1}{r_{ee}^3}\rangle$ is singular, i.e., it contains the regular and non-zero divergent parts. A general theory of singular exponential integrals was developed in our earlier works (see, e.g., [13] and references therein). In particular, in [13] we have shown that the $\langle\frac{1}{r_{ee}^3}\rangle$ expectation value is determined by the formula

$$\left\langle\frac{1}{r_{ee}^3}\right\rangle = \left\langle\frac{1}{r_{ee}^3}\right\rangle_R + 4\pi\langle\delta(\mathbf{r}_{ee})\rangle \quad (18)$$

where $\langle\frac{1}{r_{ee}^3}\rangle_R$ is the regular part of this expectation value and $\langle\delta(\mathbf{r}_{ee})\rangle$ is the expectation value of the electron-electron delta-function. Briefly, we can say that the overall contribution of the singular part of the $\frac{1}{r_{ee}^3}$ operator is reduced to the expectation value of the corresponding

delta-function. An analogous formula can be written for the $\langle \frac{1}{r_{eN}^3} \rangle$ expectation value. By using the data from Table VII we determine the lowest order QED corrections ΔE^{QED} for the ground 1^1S -states in the $^\infty\text{Li}^+$, $^\infty\text{Be}^{2+}$, $^\infty\text{B}^{3+}$ and $^\infty\text{C}^{4+}$ two-electron ions. These values are: $\Delta E^{QED}(\text{Li}^+) = 1.102\,475\,518 \cdot 10^{-4} \text{ a.u.}$ (or $7.253\,938\,191 \cdot 10^5 \text{ MHz}$), $\Delta E^{QED}(\text{Be}^{2+}) = 3.303\,586\,656 \cdot 10^{-4} \text{ a.u.}$ (or $21.736\,555\,344 \cdot 10^5 \text{ MHz}$), $\Delta E^{QED}(\text{B}^{3+}) = 7.581\,229\,698 \cdot 10^{-4} \text{ a.u.}$ (or $49.882\,095\,145 \cdot 10^5 \text{ MHz}$) and $\Delta E^{QED}(\text{C}^{4+}) = 14.744\,207\,461 \cdot 10^{-4} \text{ a.u.}$ (or $97.012\,224\,754 \cdot 10^5 \text{ MHz}$). To re-calculate the data from atomic units to MHz we used the most recent conversion factor from a.u. to MHz which equals $6.579\,683\,920\,729 \cdot 10^9$.

For two-electron ions with finite nuclear mass we need to evaluate the corresponding recoil correction to the lowest-order QED correction. Such a correction is also given in [8]. In atomic units it is written in the following form

$$\begin{aligned} \Delta E_M^{QED} = & \Delta E_\infty^{QED} - \left(\frac{2}{M} + \frac{1}{M+1} \right) \Delta E_\infty^{QED} + \frac{4\alpha^3 Q^2}{3M} \left[\frac{37}{3} - \ln \alpha - 4 \ln K_0 \right] \langle \delta(\mathbf{r}_{eN}) \rangle \\ & + \frac{7\alpha^3}{3\pi M} \langle \frac{1}{r_{eN}^3} \rangle \end{aligned} \quad (19)$$

where $M \gg m_e$ is the nuclear mass. All expectation values in this equation must be determined for the real two-electron ions which have the finite nuclear masses. The inverse mass $\frac{1}{M}$ is a small dimensionless parameter which for the ions considered in this study is $\leq 1 \cdot 10^{-4}$. By using our expectation values for the electron-nucleus and electron-electron delta-functions and for the corresponding Araki-Sucher terms ($\langle \frac{1}{r_{eN}^3} \rangle$ and $\langle \frac{1}{r_{ee}^3} \rangle$) we have determined the lowest order QED corrections for each of the ions considered in this study. Numerical values of these lowest-order QED corrections (in atomic units) can be found in Table VIII.

VII. CONCLUSION

We have performed highly accurate computations of the ground 1^1S -states in four two-electron, light ions: Li^+ , Be^{2+} , B^{3+} and C^{4+} . The results of our calculations allow us to evaluate (to very high accuracy) the non-relativistic isotopic shifts for a number of isotopes of these ions. The expectation values of different operators, which are needed during this procedure, have been determined to very high accuracy and allow one to evaluate the non-relativistic isotopic shifts for all isotopes of the two-electron, light ions discussed in this study. The lowest-order QED corrections (Quantum Electrodynamics corrections) have been also

evaluated to high numerical accuracy for each isotope of the four two-electron ions. We also discuss formulas which will be used in our next study to perform numerical calculations of the lowest-order relativistic corrections for the ground states of these two-electron ions. Future plans also include improvement of our old method which was used earlier for numerical calculations of Bethe logarithm.

Appendix. Weizäcker mass formula

The formula which provides a uniform relation between the nuclear mass M and total number of nucleons A , nuclear charge Z (= number of protons N_p) and number of neutrons N_n in the nucleus was derived in 1937 by Bethe, Weizäcker and others (known as the Weizäcker formula [14], or Bethe-Weizäcker formula). This five-term formula for the nuclear binding energy E_b was produced 75 years ago and since then its general structure has never been changed. First, note that the mass formula for an arbitrary nucleus can be written in the form

$$M = m_p \left[Z + N \left(\frac{m_n}{m_p} \right) - \frac{E_b}{m_p c^2} \right] \quad (20)$$

where M is the nuclear mass of the nucleus with A nucleons, Z protons and N neutrons, i.e. $A = Z + N$. Also in this formula E_b is the binding energy of the nucleus, c is the speed of light in vacuum, while m_p and m_n are the masses of the proton and neutron, respectively. Based on the results of most recent experiments we have for the factors $m_p c^2 = 938.272910 \text{ MeV}$ and $m_n c^2 = 939.565378 \text{ MeV}$. The advantage of the formula, Eq.(20), is obvious, since it contains only dimensionless ratios and two integer numbers (Z and N). For instance, if we choose in Eq.(20) $m_p = 1836.152701 m_e$, then M will be given in m_e (or in atomic units if $m_e = 1$). This is very convenient for highly accurate computations of different few-electron ions.

The parameter E_b in Eq.(20) is called the binding energy of the nucleus. The explicit expression for the nuclear binding energy E_b is written as the following sum (the Weizäcker formula):

$$E_b = a_V A - a_S A^{\frac{2}{3}} - a_C \frac{Z^2}{A^{\frac{1}{3}}} - a_A \frac{(N - Z)^2}{A} + \delta(A, Z) \quad (21)$$

where the five terms in the right-hand side of this equation are called the volume term, surface term, Coulomb term, asymmetry term and pairing term, respectively. The pairing

term $\delta(A, Z)$ equals zero, if A is odd. If A is even and both Z and N are even, then $\delta(A, Z) = \frac{a_p}{\sqrt{A}}$. The Weizäcker formula is relatively accurate for regular nuclei, i.e. for nuclei which are not far from the center of the stability region. In reality, such an accuracy directly depends upon the numerical values of parameters a_V, a_S, a_C, a_A and a_p in Eq.(21). To obtain the lowest-order approximation in our calculations we have used the following values of these parameters: $a_V = 15.8 \text{ MeV}$, $a_S = 18.3 \text{ MeV}$, $a_C = 0.714 \text{ MeV}$, $a_A = 23.2 \text{ MeV}$ and $a_p = 12.0 \text{ MeV}$. For all heavy nuclei and even for carbon nuclei the overall accuracy of Weizäcker mass formula is sufficient to determine the mass of the nucleus which can later be used to perform highly accurate atomic calculations. However, for Li-atoms, Be-like and B-like ions the numerical values of these parameters in the Weizäcker mass formula [14] must be modified. The reason for this follows from the fact that Weizäcker mass formula ignores the actual shell structure which is of great importance for light atomic nuclei and, therefore, it is not accurate for some light nuclei, e.g., for all nuclei of the hydrogen and helium isotopes.

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TABLE I: The total energies E and expectation values of the electron-nuclear delta-function δ_{eN} , electron-nuclear cusp ν_{eN} and some other operators for the two-electron lithium ion Li^+ (in atomic units). K is the total number of basis functions used.

K	$E(\text{Li}^+)$	$\langle\delta_{eN}\rangle$	ν_{eN}
3500	-7.279913 412669 305964 918264	6.8520 094343 431	-3.0000 00000 158
3700	-7.279913 412669 305964 918525	6.8520 094343 456	-3.0000 00000 125
3840	-7.279913 412669 305964 918626	6.8520 094343 460	-2.9999 99999 918
4000	-7.279913 412669 305964 918727	6.8520 094343 462	-2.9999 99999 901
K	$\frac{1}{2}\langle\mathbf{p}_1^2\rangle$	$\langle\mathbf{p}_1 \cdot \mathbf{p}_2\rangle$	$\frac{1}{2}\langle\mathbf{p}_N^2\rangle$
3500	3.63995 670633 465298 240	0.288975 786393 989535 661	7.56888 919906 329532 141
3700	3.63995 670633 465298 241	0.288975 786393 989535 661	7.56888 919906 329532 143
3840	3.63995 670633 465298 241	0.288975 786393 989535 662	7.56888 919906 329532 144
4000	3.63995 670633 465298 242	0.288975 786393 989535 662	7.56888 919906 329532 145

TABLE II: The total energies E and expectation values of the electron-nuclear delta-function δ_{eN} , electron-nuclear cusp ν_{eN} and some other operators for the two-electron berillium ion Be^{2+} (in atomic units). K is the total number of basis functions used.

K	$E(\text{Be}^{2+})$	$\langle\delta_{eN}\rangle$	ν_{eN}
3500	-13.65556 623842 358670 207905	17.1981 72544 645	-3.9999 99999 962
3700	-13.65556 623842 358670 207949	17.1981 72544 640	-3.9999 99999 921
3840	-13.65556 623842 358670 207968	17.1981 72544 638	-4.0000 00000 125
4000	-13.65556 623842 358670 207994	17.1981 72544 635	-4.0000 00000 148
K	$\frac{1}{2}\langle\mathbf{p}_1^2\rangle$	$\langle\mathbf{p}_1 \cdot \mathbf{p}_2\rangle$	$\frac{1}{2}\langle\mathbf{p}_N^2\rangle$
3500	6.82778 311921 179335 084	0.420520 303439 441862 011	14.07608 654186 302856 368
3700	6.82778 311921 179335 086	0.420520 303439 441862 010	14.07608 654186 302856 369
3840	6.82778 311921 179335 089	0.420520 303439 441862 009	14.07608 654186 302856 370
4000	6.82778 311921 179335 091	0.420520 303439 441862 009	14.07608 654186 302856 371

TABLE III: The total energies E and expectation values of the electron-nuclear delta-function δ_{eN} , electron-nuclear cusp ν_{eN} and some other operators for the two-electron boron ion B^{3+} (in atomic units). K is the total number of basis functions used.

K	$E(B^{3+})$	$\langle\delta_{eN}\rangle$	ν_{eN}
3500	-22.03097 1580242 781541 654073	34.758 743660 955	-5.0000 0000 319
3700	-22.03097 1580242 781541 654321	34.758 743660 965	-5.0000 0000 235
3840	-22.03097 1580242 781541 654548	34.758 743660 947	-5.0000 0000 107
4000	-22.03097 1580242 781541 654663	34.758 743660 935	-5.0000 0000 119
K	$\frac{1}{2}\langle\mathbf{p}_1^2\rangle$	$\langle\mathbf{p}_1 \cdot \mathbf{p}_2\rangle$	$\frac{1}{2}\langle\mathbf{p}_N^2\rangle$
3500	11.01548 579012 139077 100	0.552752 631642 101467 789	22.58372 421188 488300 979
3700	11.01548 579012 139077 089	0.552752 631642 101467 734	22.58372 421188 488300 952
3840	11.01548 579012 139077 086	0.552752 631642 101467 715	22.58372 421188 488300 942
4000	11.01548 579012 139077 083	0.552752 631642 101467 701	22.58372 421188 488300 938

TABLE IV: The total energies E and expectation values of the electron-nuclear delta-function δ_{eN} , electron-nuclear cusp ν_{eN} and some other operators for the two-electron carbon ion C^{4+} (in atomic units). K is the total number of basis functions used.

K	$E(C^{4+})$	$\langle\delta_{eN}\rangle$	ν_{eN}
3500	-32.40624 660189 853031 055622	61.443 578056 445	-5.9999 99998 765
3700	-32.40624 660189 853031 055638	61.443 578056 514	-5.9999 99999 871
3840	-32.40624 660189 853031 055647	61.443 578056 537	-6.0000 00000 048
4000	-32.40624 660189 853031 055660	61.443 578056 543	-6.0000 00000 037
K	$\frac{1}{2}\langle\mathbf{p}_1^2\rangle$	$\langle\mathbf{p}_1 \cdot \mathbf{p}_2\rangle$	$\frac{1}{2}\langle\mathbf{p}_N^2\rangle$
3500	16.20312 330094 926515 523	0.685334 822135 598924 527	33.09158 142403 412923 500
3700	16.20312 330094 926515 524	0.685334 822135 598924 535	33.09158 142403 412923 502
3840	16.20312 330094 926515 525	0.685334 822135 598924 536	33.09158 142403 412923 502
4000	16.20312 330094 926515 525	0.685334 822135 598924 537	33.09158 142403 412923 503

TABLE V: The nuclear radius R (fm), parameter b , factors X and Y (see the main text) and field components of the total isotopic shift ΔE_F (all values are in atomic units) for each isotope.

isotope	Q	R	b	X	Y	ΔE_F
${}^6\text{Li}$	3	2.5385	0.99976034018621	$4.297056149289 \cdot 10^{-8}$	0.81154478	$2.388077748 \cdot 10^{-7}$
${}^7\text{Li}$	3	2.4312	0.99976034018621	$4.297056149289 \cdot 10^{-8}$	0.74440369	$2.191262432 \cdot 10^{-7}$
${}^9\text{Be}$	4	2.5190	0.99957389838248	$5.749782211793 \cdot 10^{-8}$	0.79916095	$7.901106307 \cdot 10^{-7}$
${}^{10}\text{Be}$	4	2.3610	0.99957389838248	$5.749782211793 \cdot 10^{-8}$	0.70209175	$6.941535113 \cdot 10^{-7}$
${}^{10}\text{B}$	5	2.4278	0.99933413638122	$7.219245621776 \cdot 10^{-8}$	0.74241787	$1.862654830 \cdot 10^{-6}$
${}^{11}\text{B}$	5	2.4059	0.99933413638122	$7.219245621776 \cdot 10^{-8}$	0.72909310	$1.829251689 \cdot 10^{-6}$
${}^{12}\text{C}$	6	2.4073	0.99904101579314	$8.7092766851788 \cdot 10^{-8}$	0.73000871	$3.905950028 \cdot 10^{-6}$
${}^{13}\text{C}$	6	2.4614	0.99904101579314	$8.7092766851788 \cdot 10^{-8}$	0.76315629	$4.083351420 \cdot 10^{-6}$
${}^{14}\text{C}$	6	2.5037	0.99904101579314	$8.7092766851788 \cdot 10^{-8}$	0.78958608	$4.225805319 \cdot 10^{-6}$

TABLE VI: The total energies E of some isotope-substituted two-electron ions (in atomic units).
 K is the total number of basis functions used.

K	$E(^6\text{Li}^+)$	$E(^7\text{Li}^+)$
3500	-7.279223 0161006 727790 650057	-7.279321 519787 537196 699113
3700	-7.279223 0161006 727790 650265	-7.279321 519787 537196 699372
3840	-7.279223 0161006 727790 650368	-7.279321 519787 537196 699475
4000	-7.279223 0161006 727790 650468	-7.279321 519787 537196 699574
K	$E(^9\text{Be}^{2+})$	$E(^{10}\text{Be}^{2+})$
3500	-13.654709 268248 818671 527237	-13.654794 978228 935476 431692
3700	-13.654709 268248 818671 527625	-13.654794 978228 935476 435740
3840	-13.654709 268248 818671 527817	-13.654794 978228 935476 437497
4000	-13.654709 268248 818671 528033	-13.654794 978228 935476 439660
K	$E(^{10}\text{B}^{3+})$	$E(^{11}\text{B}^{3+})$
3500	-22.097340 260098 130926 358406	-22.098460 503032 611369 090170
3700	-22.097340 260098 130926 360874	-22.098460 503032 611369 092636
3840	-22.097340 260098 130926 362680	-22.098460 503032 611369 094443
4000	-22.097340 260098 130926 364302	-22.098460 503032 611369 096065
K	$E(^{12}\text{C}^{4+})$	$E(^{13}\text{C}^{4+})$
3500	-32.404733 488926 278502 692842	-32.404850 266198 080817 671544
3700	-32.404733 488926 278502 693005	-32.404850 266198 080817 671707
3840	-32.404733 488926 278502 693093	-32.404850 266198 080817 671795
4000	-32.404733 488926 278502 693224	-32.404850 266198 080817 671923
K	$E(^{14}\text{C}^{4+})$	—
3500	-32.404949 988753 619902 032262	—————
3700	-32.404949 988753 619902 032424	—————
3840	-32.404949 988753 619902 032513	—————
4000	-32.404949 988753 619902 032644	—————

TABLE VII: The expectation values of the delta-functions and other operators used in calculations of the ΔE_{∞}^{QED} and ΔE_M^{QED} corrections for the ground $1^1S(L=0)$ -state in the model two-electron ions with the infinite nuclear masses (in atomic units).

	∞Li^+	∞Be^{2+}	∞B^{3+}	∞C^{4+}
$\langle\delta(\mathbf{r}_{eN})\rangle$	6.8520 094343 462	17.1981 72544 635	34.758 743660 935	61.443 578056 543
$\langle\delta(\mathbf{r}_{ee})\rangle$	0.5337 225365 611	1.52289 53514 918	3.3124 421128 343	6.1410 439710 717
$\ln K_0$	5.1798 4912 9	5.7550 9181 3	6.2014 6720 1	6.5662 3588 3
$\langle(r_{ee}^{-3})_R\rangle$	-6.5281 0829 296	-26.725 9651 077	-70.595 6634 154	-148.72 6462 987

TABLE VIII: The expectation values which are needed to determine the mass-dependent components of the isotopic shifts and recoil correction to the lowest-order QED corrections ΔE_M^{QED} (all values are in atomic units) for each isotope.

isotope	$\frac{1}{2}\langle \mathbf{p}_1^2 \rangle$	$\langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle$	$\frac{1}{2}\langle \mathbf{p}_N^2 \rangle$
^6Li	3.63926634776862256908	0.2886900796744086288	7.56722277521165376698
^7Li	3.63936484138499574890	0.2887308379661048866	7.56746052073609638437
^9Be	6.82692618052016588002	0.4201657546934667785	14.0740181157337985385
^{10}Be	6.82701188451767303607	0.4202012115590292674	14.0742249805943753395
^{10}B	11.0142482768039452882	0.5522411301146439512	22.5807376837225345276
^{11}B	11.0143602940252942064	0.5522874275672885044	22.5810080156178769173
^{12}C	16.2016102297131475001	0.6847099993208290105	33.0879304587471240106
^{13}C	16.2017270007914486371	0.6847582175983323092	33.0882122191812295834
^{14}C	16.2018267184515755466	0.6847993943186503851	33.0884528312218014784
isotope	$\langle \delta_{eN} \rangle$	$\langle (r_{eN}^{-3})_R \rangle$	$\Delta E_M^{QED} \text{ a.u. } (\Delta E_M^{QED} \text{ MHz})$
^6Li	6.8501121960089	-238.6352250738	$1.1021361193 \cdot 10^{-4}$ ($7.2517073026 \cdot 10^5$)
^7Li	6.8503828685062	-238.6457736206	$1.1021844969 \cdot 10^{-4}$ ($7.2520256117 \cdot 10^5$)
^9Be	17.195002927213	-662.1327513745	$3.3029131600 \cdot 10^{-4}$ ($2.1736555344 \cdot 10^6$)
^{10}Be	17.195319920709	-662.1462731118	$3.3029805117 \cdot 10^{-4}$ ($2.1732567764 \cdot 10^6$)
^{10}B	34.752987732681	-1436.920035269	$7.5798489928 \cdot 10^{-4}$ ($4.9873010540 \cdot 10^6$)
^{11}B	34.753508739203	-1436.943743086	$7.5799739787 \cdot 10^{-4}$ ($4.9873832907 \cdot 10^6$)
^{12}C	61.435098004106	-2682.390222121	$1.4741983427 \cdot 10^{-3}$ ($9.6997591317 \cdot 10^6$)
^{13}C	61.435752441957	-2682.421520508	$1.4742155075 \cdot 10^{-3}$ ($9.6998720706 \cdot 10^6$)
^{14}C	61.436311305958	-2682.448248113	$1.4742301655 \cdot 10^{-3}$ ($9.6999685151 \cdot 10^6$)